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Charge fraction for positron Auger neutralization on metal surface

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Abstract : The theory for Auger neutralization of positrons at metal surfaces was developed in an earlier work Transition rate was calculated as a function of distance from surface. It was shown to decay exponentially with distance from surface. The charged fraction for positrons scattered in front of a metal surface and going through Auger neutralization is calculated in this work The charge fraction for energetic positrons from aluminum surface is found to be very high, implying a low probability of neutralization for these energetic positrons. For positrons with velocity in the parallel direction less than 0.05 atomic units, the charge fraction almost diminishes.

Keywords : Positron neutralization, charge fraction, positron-solid interaction, Auger neutralization

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Auger neutralization of low-energy ions was developed as an analytical tool in the field of surfaces electronic structure investigation [1,2]. In this process, a beam of low kinetic energy ions is scattered off a solid surface, and depending on the values of the ionization potentials of the projectiles and surface work function, Auger electrons can be emitted during the neutralization of part of the incoming ions. Charge transfer phenomena between particles and surfaces is also relevant in the field of plasma. Since some charged particles might be neutralized when colliding with the walls of the confinement method. Charge transfer is involved in many surface processes in surface chemistry. Its study should help to evaluate the reactivity and other chemical properties of a given surface. The transition rate of neutralization is a very rich quantity [3]. It gives direct information on the likelihood of a given process. It can be used in a rate equation to obtain the ion population at a given distance from the surface [1,4]. It was shown by Lorente *et al* [5] that the neutralization rate is intrinsically related to the calculation of the contribution to the electron spectra in charged particle scattering from surfaces experiments.

In a previous work [6], the interaction of positrons (positively charged particles) with metal surface that leads to neutralization was considered. And the transition rate was calculated assuming the mechanism of Auger neutralization. Here, an electron is captured into an unoccupied 'atomic' level of lower energy forming a bound particle, the positronium. The energy of the transition is used for exciting the surface or more specifically, an electron on the surface. This excited electron is to be called Auger electron if its excitation energy is such that it is able to escape the surface potential. The open (the energetically allowed) neutralization channels are determined by the position of the Fermi level with respect to the relevant empty atomic level of the scattered particle.

Since the advances made in the production of intense positron beams and the better understanding of positron surface interaction, the importance of this field has grown rapidly [7–9]. Positrons are now used in many ways to probe surfaces [10]. Low energy positron diffraction (LOPD), reflection high energy positron diffraction (RHEPD) and positron-annihilation induced Auger electron spectroscopy (PAES) are now part of the experimental methods for surface analysis [11–13]. In PAES, which was developed since the late 1980s by Weiss and co-workers, Auger electron emission results from annihilation

of a surface core electron by a positron implanted with very low energy [14,15]. Of course, positronium is formed at the surface of metals when the electron density is low enough to allow single electron-positron pairing. Positronium formation has the potential to be exploited as a probe of surface electronic structure. With the assumption that positronium formation is sudden, the velocity distribution of positroniums formed should yield information on the electronic density of states.

Positronium represents a bound state between a positron and an electron. It can be treated formally as a hydrogen atom. The ionization energy of positronium is half of that of hydrogen, being 6.8 eV, and its radius is double that of hydrogen, being 1.02 Angstrom. The positronium is usually formed when a high energy free positron is slowed down to the point where it is energetically favorable to ionize an electron off a nearby atom or a conduction band of a solid and bind with it. However, if the positron is too slow it will not have enough energy to ionize an electron and will annihilate with whatever electron happens to be nearby. Since the positronium state is unstable inside bulk metals it is formed from positrons that do not penetrate the surface.

From experimental point of view, there are two advantages for studying positron neutralization over ion neutralization. First, it is easy to measure the neutral fraction, which is defined to be the ratio of created positronium flux over the positron flux. This is because positronium decays into gamma-rays. The second is the fact that the positronium momentum distribution spreads out and reflects the electronic momentum distribution of the surface.

In my previous paper [6], I have proposed the process of Auger neutralization for positron scattering from metal surface. This was made on the assumption of similarity between ion and positron scattering from solid surfaces. Both particles, ion and positron, are charged particles that present the same potential disturbance when appear close to the metal surface. The main difference might be the small mass of the positron compared to the ion and the fact that in the positronium bound state, the positron and electron orbit each other. The theory developed therein takes into account the motion of the incoming positron and the orthogonalization of the bound positronium atomic state with the metal electronic states. The calculated transition rate (a measure of the probability of neutralizing an incoming positron) decays exponentially with distance from the surface. A local maximum value at distance of 1.3 (in atomic units) was attained. A local minimum at distance of 1 (in atomic units) was also noticed. This was explained in terms of the repulsive potential of the positive background of the metal.

Neutral fraction or consequently charged fraction presents a good test for the theory of charged particle neutralization. The charged fraction Φ^+ is defined as the ratio of the scattered charged particle flux (N^+) to the total scattered flux (N^{total}).

$$\Phi^+ = \frac{N^+}{N^{\text{total}}} \tag{1}$$

and similarly, the neutral fraction Φ^0 is defined to be

$$\Phi^0 = \frac{N^0}{N^{\text{total}}} \tag{2}$$

Here, N^0 is the flux of neutralized particles. Of course, the condition $F^+ + F^0 = 1$ must be met. As is assumed in most of theoretical calculations for neutral fraction [16–22], a classical trajectory for the charged particle is assumed. Specular reflection and constant charged particle velocity $v_\perp$ in the perpendicular direction is also used. Within these assumptions, the charged particle flux assumes the simple relation

$$\Phi^+(s) = \Phi^0 \exp\left[-\frac{1}{v_\perp}\int T(s')ds'\right] \tag{3}$$

In eq. (3), $T(s)$ is the calculated transition rate for the process and s is the distance from the surface. The limits of the integral are such that it allows the neutralization to occur at a distance s at any point in the trajectory of the charged particle. In eq. (3) the value of the integral over the transition rate over the trajectory of the positron is calculated using the results in [6]. It is represented as a parameter v_c usually called characteristic velocity. Large values for v_c (characteristic velocity) correspond to strong neutralization. The charge fraction relation will then take the simple form :

$$\Phi^+ = e^{-(v_c/v_\perp)}. \tag{4}$$

In curve (a) of Figure 1, the charge fraction for positrons scattered from aluminum surface is plotted against the incident positron velocity $v_\perp$ in the perpendicular to the surface direction. The values of the velocities are in atomic units. The figure shows that the charge fraction is almost zero for positron velocities below 0.05. This implies that for these positrons, total neutralization is expected. Of course, this is understood with the realization of the fact that the positrons will

spend more time in front of the surface and consequently, will have a higher probability to be neutralized. The

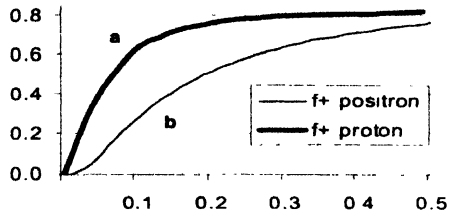

Figure 1. Charge fraction for Auger neutralization against positrons velocities perpendicular to the surface direction $v_\perp$ (atomic units for velocities are used). Curve (a) represents the case of protons scattered from aluminum surface. Curve (b) represents the case of positrons scattered from aluminum surface.

charge fraction will reach a high value for very energetic positrons. The maximum value of $v_\perp$ assumed is 0.5, since more energetic positrons will have a high probability of entering into the surface which is not taken into account in this theory. In fact, the smallest value of distance from surface taken in the integral in eq. (3) is 3 (1.5 Å). This is to allow the bound positronium state to be outside the surface.

For the sake of comparison, curve (b) in the figure exhibits the charge fractions for protons scattered from aluminum surface against velocity perpendicular to the surface direction, in addition to the case of positron Auger neutralization. The results for protons neutralization by Auger mechanism is taken from a previous work [23]. It is clear from the figure that the charge fraction for protons is greater than that for positrons. This implies that for the same incident energy, positrons will have a higher probability of neutralization by Auger mechanism than for protons that have the same velocity in the perpendicular to the surface direction. From the figure, the characteristic velocities v_c as defined in eq. (4) for proton and positron neutralizations are extracted to be 0.138 and 0.05 consequently. The characteristic velocity for Auger positron neutralization is higher than Auger proton neutralization.

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